Molecular Electronics: Structural Contribution to Charge Transport across Ni-Octanedithiol Multilayer Junctions

NIST researchers have focused on applying an electronically based spectroscopic technique on novel molecular systems to gain fundamental understanding to the functional mechanism for molecular electronic devices. The ability to identify reliably the origin of the electrical transport characteristics of any given molecular-based device is one of the critical technical goals that many in the field of molecular-based electronics are endeavoring to accomplish.

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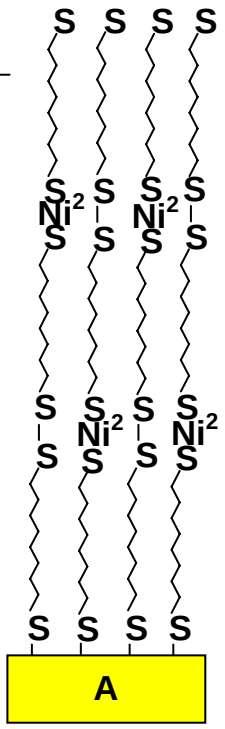
This research demonstrates that the electrical transport through these molecular multilayer junctions is dominated by the intrinsic properties of the multilayer.

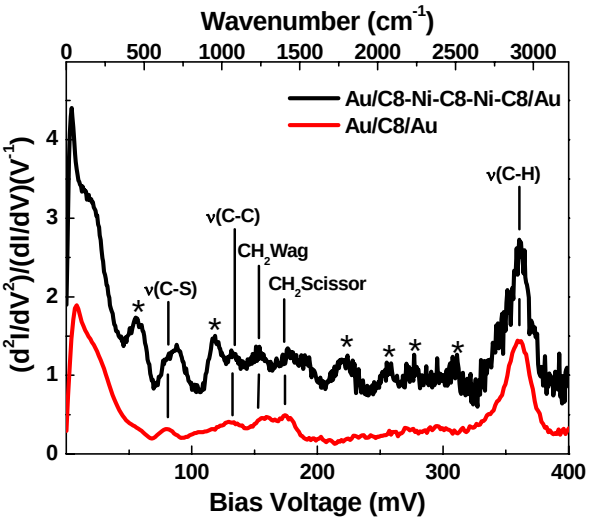
Molecular-based electronics have the potential to become a complementary or even the replacement technology for the semiconductor-based electronics we use today. One of the barriers to this innovation is the ability to identify reliably the origin of the electrical transport characteristics of any given molecular-based device.

The NIST team has demonstrated that the transport characteristics of a molecular junction can be directly influenced by the active design of the molecular components. Using 1,8-octanedithiol **(C8)** and Ni(II) ions as the molecular building blocks, we employ a bottom-up approach to assemble molecular multilayer structures, which exhibit electrical transport behavior commensurate with their structural design. The structures of the multilayers, were determined by ellipsometry, Fourier transform infrared spectroscopy and X-ray photoelectron spectroscopy. A schematic of the resultant multilayer is given in the figure.



The electrical transport measurements of these molecular devices were performed with a custom-built cryogenic cross-wire tunneling junction apparatus, and the vibrational modes of the multilayer were measured electronically by the inelastic electronic tunneling (IET) spectroscopy. In these molecular devices we observe vibrational excitations that match the known and calculated vibrational spectra of the molecular multilayer. The figure shows the IET spectra of **C8** monolayer and **C8**/Ni(II) multilayer, along with mode/vibrational assignments. A number of these devices also exhibit stochastic gating due to time varying charging of defects in the molecular multilayer.

Figure 1: ***(Left) Schematic structure of C8/Ni(II) multilayer. (Below) Inelastic electron tunneling spectra of a C8-Ni-C8-Ni-C8 multilayer junction (black) and a C8 monolayer junction (red). The black trace is shifted vertically by 0.5 V^{-1} for clarity. Mode assignments are from comparison to previous experimental results and density functional theory calculations. The asterisks mark the IETS mode observed only in the molecular multilayer junction.***



Future Plans: We plan to investigate the magnetic and magnetoresistive properties of these multilayer structures. One goal of this project is to understand how an external magnetic field can influence the electrical transport behavior of a molecular device that is incorporated with ferromagnetic ions.

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